SCATTERING S-WAVE ELECTRONS OFF ATOMIC HYDROGEN

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THESIS

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ABSTRACT

The Kohn variational method of calculating scattering phase shifts has been examined previously, and calculations of the phase shifts of S-wave electrons on atomic hydrogen done, by Schwartz. This paper presents the results of using a trial function somewhat simpler than Schwartz's and compares the two sets of results. In addition this paper presents and compares the results of two different normalizations of the variational principle and gives a somewhat more detailed development of the variational principle used than in most previous papers.

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I. INTRODUCTION

In 1961 Schwartz used Kohn's variational principle to calculate the scattering phase shift of S-wave ($\ell = 0$) electrons incident on atomic hydrogen. The trial wave function he used had the form

$$\Psi = \phi + \sum_{\ell mn} C_{\ell mn} e^{-k/2(r_1+r_2)} r_{12}^{\ell} \left(r_1^m r_2^n \pm r_1^n r_2^m \right) / 4\pi\sqrt{2}$$

where $$\phi = (1 \pm \hat{P}_{12}) 2 e^{-r_2} \left[\frac{\sin kr_1}{kr_1} + \tan(\eta) \frac{\cos kr_1}{kr_1} \right.$$

$$\left. (1 - e^{-k/2 r_1}) \right] / 4\pi\sqrt{2}$$

with as many as 50 terms in the sum [Ref. 1].

This paper presents the results of calculations for the same problem using a different trial wave function. Assuming the results of Schwartz's calculations are correct, a comparison of the new results to his is made to determine the relative merits of the new trial wave function. The new calculations were also done using two different normalizations of the variational principle, and a comparison between these results is also presented. As a lead-in to the actual calculations this paper first presents a development of the theory behind them.

II. THEORY

A. VARIATIONAL THEORY

1. General Form

First in the presentation of the theory is a general look at the variational method of determining the exact wave function of a system. The general variational principle starts with the integral

$I = \frac{2m}{\hbar^2} \int \Psi(E-\hat{H})\Psi \, d\tau$ which equals 0 when Ψ is the exact wave function. After some manipulation it is found (See Appendix A-1), in spherical coordinates, that

$$\delta I = 2\frac{2m}{\hbar^2} \int \delta\Psi(E-\hat{H})\Psi \, d\tau + \lim_{r\to\infty} \int_S r^2 \Psi \frac{d}{dr}\delta\Psi \, d\Omega$$

$$- \lim_{r\to\infty} \int_S r^2 \delta\Psi \frac{d}{dr}\Psi \, d\Omega$$

or $$\delta I = \lim_{r\to\infty} \left[\int_S r^2 \Psi \frac{d}{dr}\delta\Psi \, d\Omega - \int_S r^2 \delta\Psi \frac{d}{dr}\Psi \, d\Omega \right]$$

when Ψ is the exact solution of $\hat{H}\Psi = E\Psi$.

2. Specific Forms

Now, by specifying the radial portion of Ψ at $r = 0$ and as $r\to\infty$ the general result above yields a particular variational principle. For example, the necessary conditions imposed on Ψ for a bound state of angular momentum ℓ are that at $r = 0$ $\chi_\ell(r) = 0$ where $\Psi = \frac{\chi_\ell(r)}{r} \Phi(\theta,\phi)$ and that as $r\to\infty$ $\Psi\to 0$. These give $\delta I = 0$ which is the Rayleigh-Ritz variational principle for bound states. The Kohn variational method for scattering phase shifts is derived from this general formula by putting in a set of conditions appropriate to the scattering problem. Therefore an examination of the appropriate conditions is now presented.

B. SCATTERING THEORY

1. Phase Shifts and Partial Wave Analysis

First note that the phase shift being calculated is the phase difference between the radial portions of the asymptotic forms of the wave functions with the scattering potential and without the scattering potential. Dividing the incoming wave into partial waves by angular momentum (partial wave analysis) there exists a phase shift for each partial wave. This set of phase shifts completely determines the scattering cross section. In the case of low energy scattering all the phase shifts, except the S or $\ell = 0$ wave phase shift, are very small, and therefore the S-wave phase shift is often the only one needed for accurate calculations.

2. Asymptotic Conditions

So the conditions needed are those on the radial portion of the solution for angular momentum ℓ of $(E - \hat{H})\Psi = 0$ in spherical coordinates where $\hat{H}$ is the Hamiltonian with the scattering potential included. At $r = 0$ the radial portion $R_\ell(r) = \frac{\chi_\ell(r)}{r}$ must be finite which implies that χ_ℓ must equal 0. As $r \to \infty$, and the potential approaches 0, Ψ must become like the wave function of a free particle, and the most general form χ_ℓ can assume in spherical coordinates is shown by Schiff [Ref. 2] to be $\chi_\ell(r) \xrightarrow[r\to\infty]{} \frac{f(\eta_\ell)}{k} \sin(kr - \frac{\ell\pi}{2} + \eta_\ell)$ where η_ℓ is the phase shift of the ℓ^{th} partial wave, and $f(\eta_\ell)$ is an arbitrary amplitude function.

C. FINAL VARIATIONAL PRINCIPLE

1. Final Form and Normalization

Putting these conditions into the general form and allowing η_ℓ to be the variable parameter for $\delta\Psi$ yields the specific form

$$\delta I = -f^2(\eta_\ell)/k \quad \delta\eta_\ell$$ (See Appendix A-1).

Now choose $f(\eta_\ell) = \text{secant}(\eta_\ell)$ and write $F(\eta_\ell) = \int f^2(\eta_\ell)\, d\eta_\ell$ so that $f^2(\eta_\ell)\,\delta\eta_\ell = \delta F(\eta_\ell)$ and $\delta I = -\delta F(\eta_\ell)/k = \frac{-\delta\tan(\eta_\ell)}{k}$. Then $\delta\left(I + F(\eta_\ell)/k\right) = \delta\left(I + \tan(\eta_\ell)/k\right) = 0$ which is Kohn's variational principle.

Ordinarily Kohn's principle is written $[\tan(\eta_\ell)/k] = I + \frac{\tan(\eta_\ell)}{k}$ which means that when Ψ is exact $I + \tan(\eta_\ell)/k = \tan(\eta_\ell)/k$ So by taking the variation of $I + \frac{\tan(\eta_\ell)}{k}$ with respect to several variable parameters in a trial function Ψ, one of which is η_ℓ, and finding the values of these parameters which make $I + \frac{\tan(\eta_\ell)}{k}$ stationary, $\delta(I + \tan(\eta_\ell)/k) = 0$, one gets first order values of η_ℓ and the other parameters. These first order values are then substituted back into $I + \frac{\tan(\eta_\ell)}{k}$ to give the stationary result $[\tan(\eta_\ell)/k]$.

2. Usefulness of Variational Theory

What good is all this? It means that to find the scattering phase shifts all one has to do is select a reasonable trial wave function with several variable parameters which satisfies the above conditions, put it in the integrals, find parameter values that satisfy $\delta(I+\tan(\eta_\ell)/k) = 0$ and put these values back into $[\tan(\eta_\ell)/k] = I+\tan(\eta_\ell)/k$ If one can find a relatively simple and easy-to-integrate wave function that gives good results for a difficult problem, this method may save considerable work. This is a big if with complications.

III. CALCULATIONS

A. GENERAL OUTLINE

In the case of variational calculations of scattering phase shifts a unique problem appears. In scattering calculations $E - \hat{H}$ has a continuum of eigenvalues which passes through 0. In the calculations $E - \hat{H}$ is represented by a matrix M_{ij} in the subspace of the complete Hilbert space of $\hat{H}$ which is spanned by the N terms in the trial function. This matrix has N eigenvalues and when any of these eigenvalues becomes very small $\tan(\eta_\ell)/k$ may become very large and inaccurate. Thus at a given energy E convergence to better values with more terms is not guaranteed. However, by adding a non-linear variable κ to the trial wave function and varying it for each value of E the behavior of $\tan(\eta_\ell)/k$ can be mapped out. Then the best value of $\tan(\eta_\ell)/k$ is found by picking the value from the flattest part of the graph of $\tan(\eta_\ell)/k$ versus κ. As the trial wave function becomes more and more accurate with more and more variable parameters the flat regions of the curve become flatter and longer; converging, hopefully, to better and better values of the phase shift. When the improvement becomes small compared to the size of $\tan(\eta_\ell)/k$ the final value is determined from the flat region of the graph and the probable further improvement due to more terms. The error is estimated from reading the graph and how well the further improvement can be determined. A good presentation of this general method of calculation is given in Schwartz [Ref. 3]. The method used in the present case differs by using the values from the curves directly without estimating probable improvement and estimating the error only from reading the graph.

B. THE HAMILTONIAN

Now apply the above to scattering S-wave electrons off atomic hydrogen. In this problem there is an incoming electron, the hydrogen proton and the electron bound to the proton, all of which interact with one another. To take in all these interactions the following Hamiltonian was used

$$\frac{2m}{\hbar^2}[E-\hat{H}] = k^2 - 1 + \nabla_1^2 + \nabla_2^2 + \frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}}$$

where radial distance and energy are in Bohr radii and Rydberg units respectively (See Appendix B). Therefore k^2 is the energy of the incoming electron, and -1 is the energy of the bound electron in the ground state. To avoid the complications of excitation of the bound electron k was limited to less than .866, which corresponds to about 10.2 ev, so only low energy scattering was considered.

C. THE TRIAL WAVE FUNCTION

However one still had to take into account the indistinguishability of the electrons, and this was done with the trial wave function. The following wave function was used

$$\Psi = \phi + \sum_{jm} \left(\frac{\kappa}{2}\right)^{j+m} C_{jm} e^{-\kappa(r_1+r_2)} (r_1^j r_2^m \pm r_1^m r_2^j) \frac{2}{4\pi\sqrt{2}}$$

$$\phi = \frac{2}{4\pi\sqrt{2}} (1 \pm \hat{P}_{12})[j_0(kr_1) - \tan(\eta)\, j_1(kr_1)]\, e^{-r_2}$$

where $\hat{P}_{12}$ is the parity operator that interchanges r_1 and r_2 and where $j_0(kr_1) = \frac{\sin kr_1}{kr_1}$ and $j_1(kr_1) = \frac{\sin kr_1}{(kr_1)^2} - \frac{\cos kr_1}{kr_1}$ are spherical Bessel functions. The + sign gives a symmetric wave function which

implies spin angular momentum S = 0, and the - sign gives an anti-symmetric wave function which implies S = 1. Thus the $1 - \hat{P}_{12}$ takes care of the indistinguishability of the electrons and their fermion properties.

is the asymptotic part of the wave function and approaches

$$\frac{\sqrt{2}}{4\pi}\,\text{secant}(\eta)\,\frac{\sin(kr_1+\eta)}{kr_1}\,e^{-r_2} \qquad \text{as } r_1\to\infty$$

and $$\frac{\sqrt{2}}{4\pi}\,\text{secant}(\eta)\,\frac{\sin(kr_2+\eta)}{kr_2}\,e^{-r_1} \qquad \text{as } r_2\to\infty$$

contains the necessary asymptotic plane wave condition for one electron, coupled with a ground state condition for the other electron in the e^{-r} term. The sum portion contains the close-in terms with the variable parameters C_{jm}. Note that η is also a variable parameter.

D. INTEGRALS AND FINAL FORMULAS

Now with two electrons two radial coordinates, r_1 and r_2, and their difference, r_{12}, are used. Does this change the variational principle? The answer is no, with the proper normalization of the trial wave function (See Appendix A-2). So the variational principle remains $[\tan(\eta_e)/k] = I + \tan(\eta_e)/k$. Now defining

$$\Psi = \phi + \sum_i C_i \chi_i\,,\quad \lambda = \tan(\eta)\,,\quad C_i = C_i^{\circ} + \lambda C_i^{1}$$

$$B = \frac{2m}{\hbar^2}\int \phi(E-\hat{H})\phi\, d\tau_1 d\tau_2 = B_0 + \lambda B_1 + \lambda^2 B_2$$

$$R_i = \frac{2m}{\hbar^2}\int \chi_i(E-\hat{H})\phi\, d\tau_1 d\tau_2 = R_i^{\circ} + \lambda R_i^{1}$$

$$M_{ij} = \frac{2m}{\hbar^2}\int \chi_i(E-\hat{H})\chi_j\, d\tau_1 d\tau_2$$

one solves $\frac{\partial}{\partial C_i}(I + \lambda/k) = \sum_j M_{ij} C_j + R_i = 0$ and

$\frac{\partial}{\partial \lambda}(I + \lambda/k) = 0$ to get the C_i and λ to first order. Then inserting these values back into the variational equation gives

$$[\lambda/k] = W_0 + B_0 - \frac{(W_1 + B_1 + 1/k)^2}{4(W_2 + B_2)}$$

where $W_0 = \sum_i C_i^0 R_i^0$, $W_1 = 2\sum_i C_i^1 R_i^0$, and $W_2 = \sum_i C_i^1 R_i^1$ as shown by Schwartz [Ref. 3] . These are the final integrals and equations used in the calculation of the phase shift using $f(\eta) = \text{secant}(\eta)$. The phase shift was also calculated using $f(\eta) = \text{cosecant}(\eta)$ which gives

$[-\cot(\eta)/k] = I - \cot(\eta)/k$ and requires

$$\phi = \frac{\sqrt{2}}{4\pi}(1 \pm \hat{P}_{12})\left[\cot(\eta) j_0(kr_1) - j_1(kr_1)\right] e^{-r_2}$$

The final formula is

$$[-\lambda/k] = W_2 + B_2 - \frac{(W_1 + B_1 - 1/k)^2}{4(W_0 + B_0)}$$

where $\lambda = \cot(\eta)$ and the W's and B's remain the same as before except $B = \lambda^2 B_0 + \lambda B_1 + B_2$, $C_i = \lambda C_i^0 + C_i^1$, and $R_i = \lambda R_i^0 + R_i^1$.

E. THE ACTUAL CALCULATIONS

The actual calculations are done as follows. First the integrals B_0, B_1, B_2, R_i^0, R_i^1, M_{ij} are done by hand for the general case, and then the final numbers are obtained by computer evaluation of the general integrals for particular cases. Then $\sum_j M_{ij} C_j = -R_i$ is solved independently of the first order solution for λ since $C_j = C_j^0 + \lambda C_j^1$ and M_{ij} independent of λ implies $\sum_j M_{ij} C_j^0 = -R_i^0$, and $\sum_j M_{ij} C_j^1 = -R_i^1$. This solution is most accurately done by matrix inversion. The $\left(\frac{k}{2}\right)^{l+m}$

factors in the close-in terms of Ψ are there to increase the accuracy of the matrix inversion and have no effect on the value of the phase shift. Finally the W's and the stationary value of $\frac{\lambda}{k}$ are calculated using the previously given formulas.

The above calculations were done for values of κ from 0.6 to 2.5 in steps of 0.1 for each value of k from 0.1 to 0.8 in steps of 0.1 with up to 40 close-in terms. This was done for both the symmetric and antisymmetric wave functions and both secant and cosecant normalizations. Then the values of $\tan(\eta)/k$ or $-\cot(\eta)/k$ were plotted versus κ for each case by the computer (See Figs. 1, 2, 3, 4), and values of $\tan(\eta)/k$ and $-\cot(\eta)/k$ selected from the flattest portion of each curve. The actual values of η were then calculated from these numbers for comparison with Schwartz's values. Additional values were obtained for $k = 0.4$ at 49, 56, and 72 terms to see how much better the values might get and where significant inaccuracies in the matrix inversion would occur.

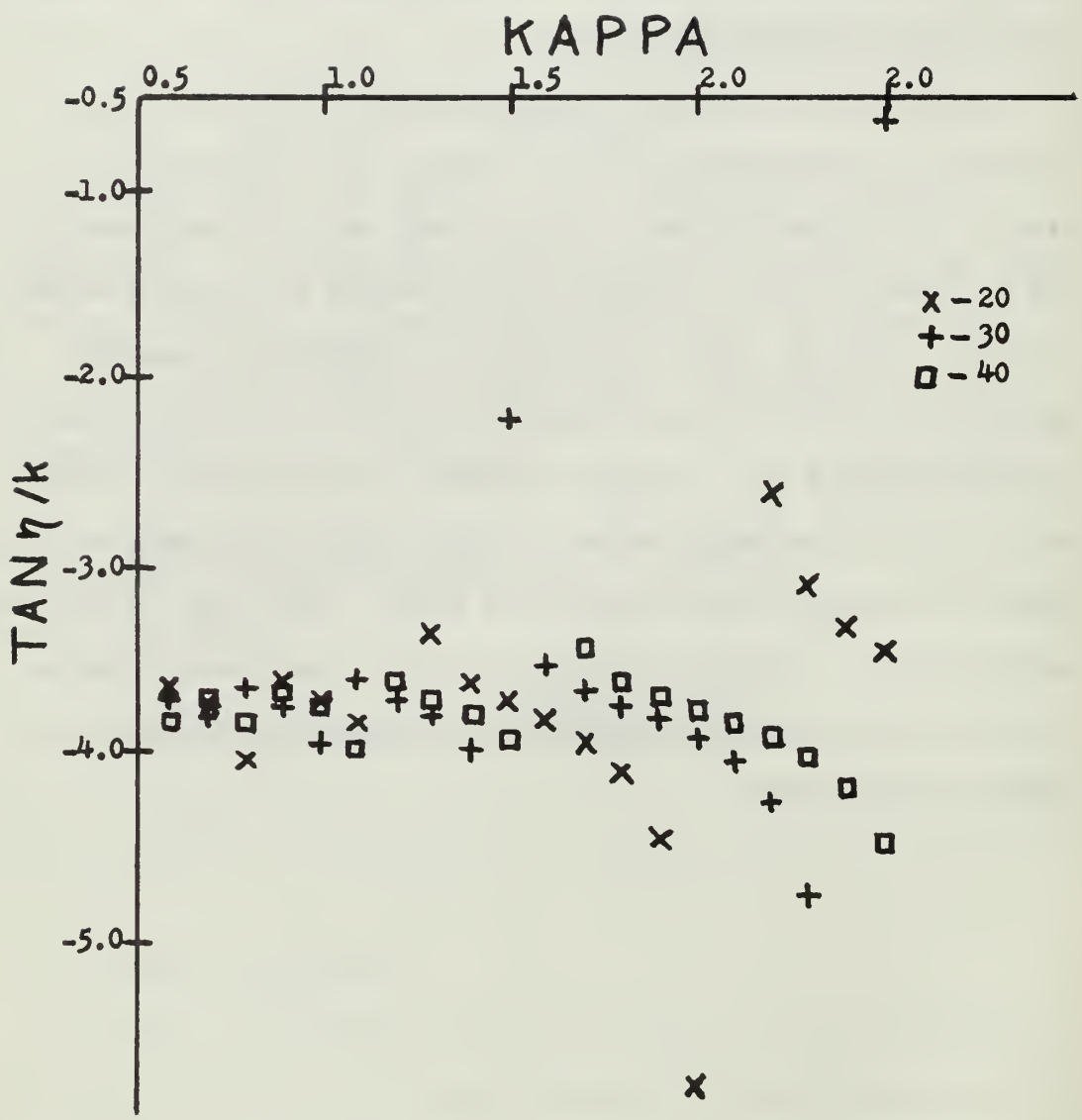

Fig. 1 - Graph of tan(η)/k versus κ (kappa) for k=0.5 and S = 1.

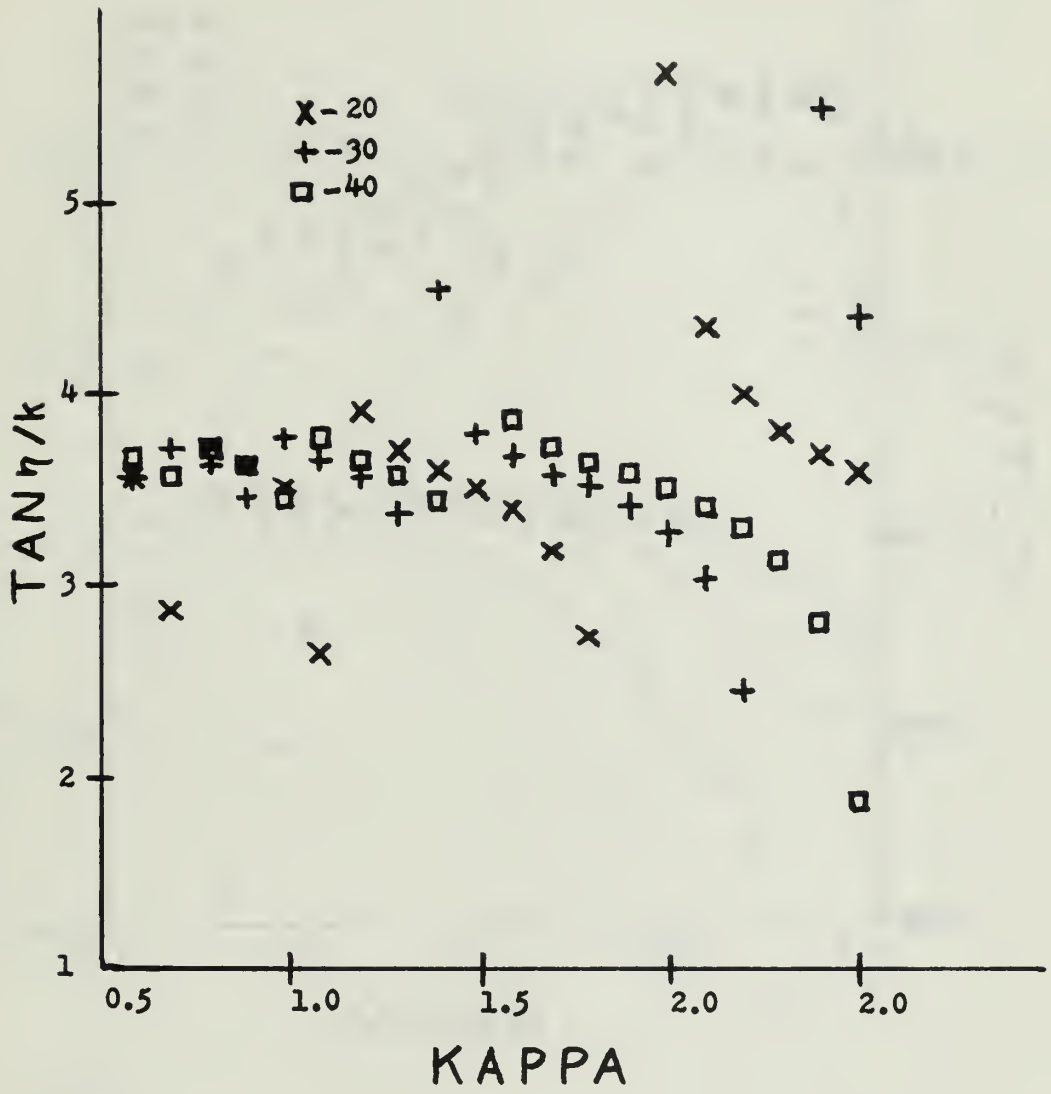

Fig. 2 - Graph of $\tan(\eta)/k$ versus κ (kappa) for $k = 0.5$ and $S = 0$.

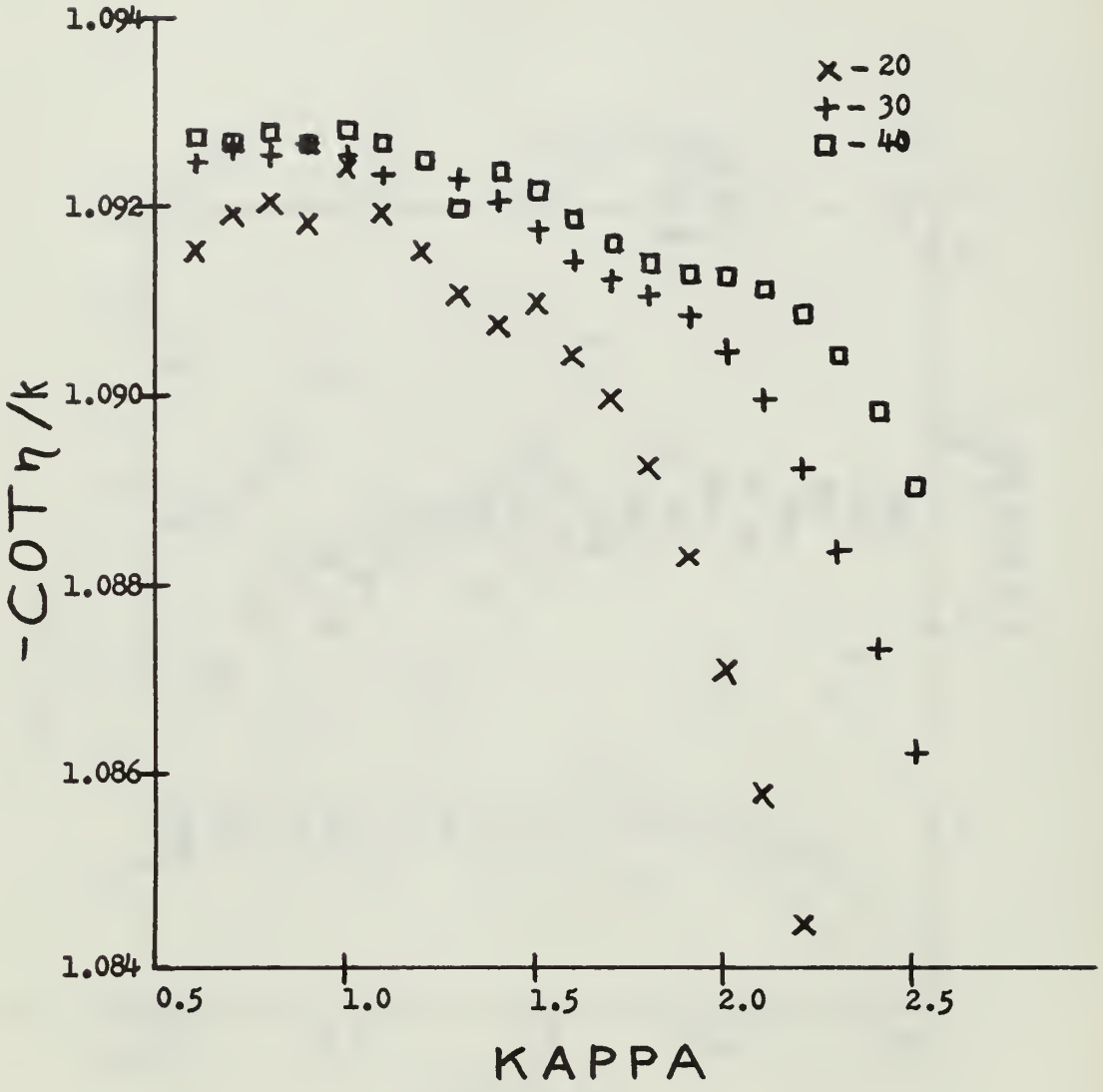

Fig. 3 - Graph of $-\cot(\eta)/k$ versus k (kappa) for $k = 0.5$ and $S = 1$.

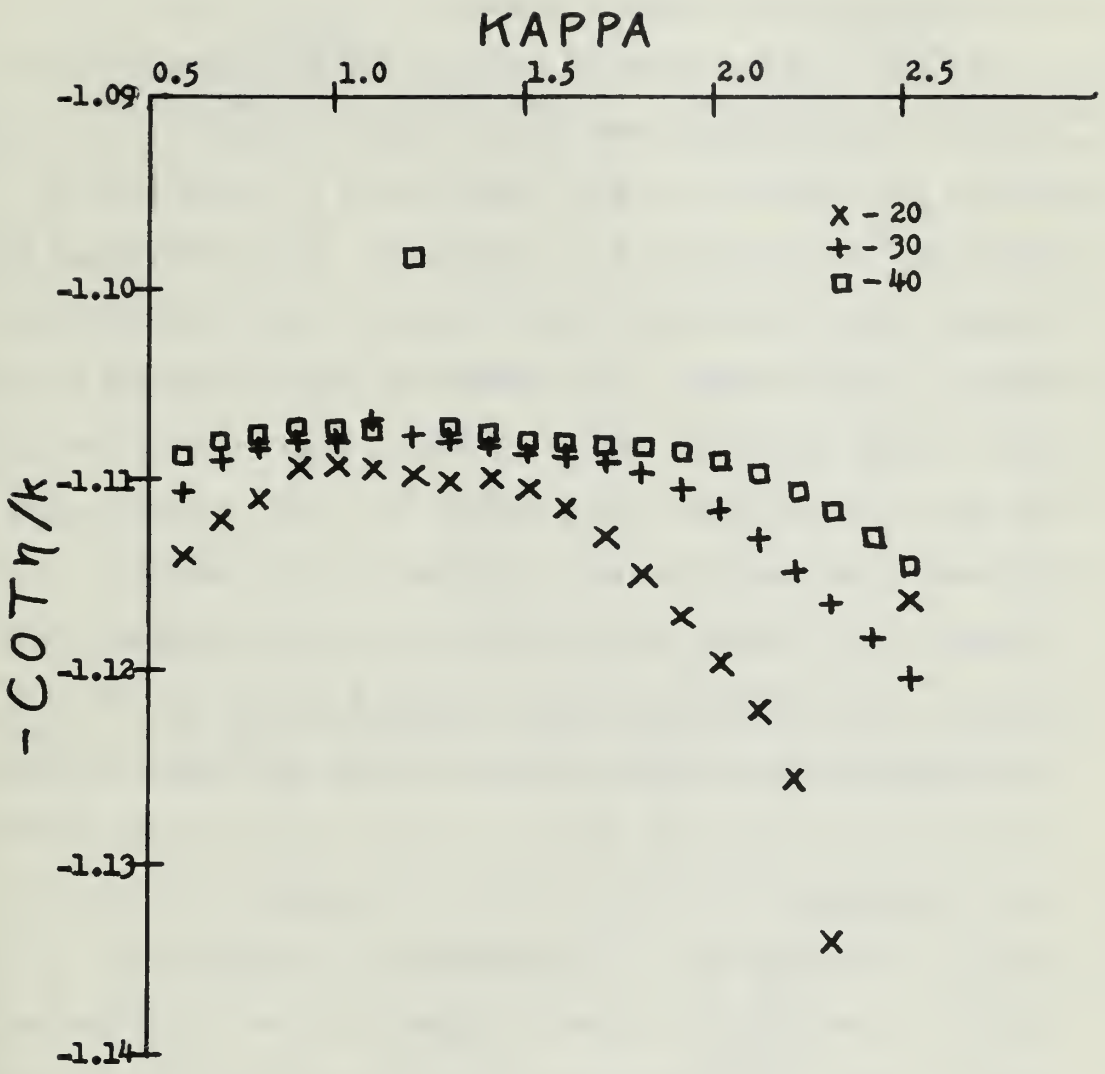

Fig. 4 - Graph of $-\cot(\eta)/k$ versus κ (kappa) for k= 0.5 and S=0.

IV. DISCUSSION OF RESULTS

A. COMPARISON WITH SCHWARTZ'S RESULTS

Table I lists the values of $\tan(\eta)/k$ and η obtained from the present calculations and from Schwartz's calculations for S = 1. Table II does the same for S = 0 and Tables III and IV do the same for $-\cot(\eta)/k$ for S = 1 and S = 0 respectively. The uncertainties in the present values listed in the tables represent the errors one would estimate from the graphs in the absence of Schwartz's values for comparison. Comparison of the results is done quite easily from the tables, and the following results are obtained. In Table I the percentage differences between the values of present calculations for η and Schwartz's calculations are between 2% and 8% with one case of 12%. In Table II the differences in η are between 10% and 20% with one case of 40% and one of 207%. In Table III the differences in η are between 2% and 8% with one case of 15%, and in Table IV the differences are between 9% and 20% with one case of 30% and one of 213%. In the cases with 207% and 213% differences in η the differences in the absolute values are only 2% and 9% respectively but the values have opposite signs. These two cases are the only such cases of difference in sign, both occur at $k = 0.3$ for S = 0, and neither can be explained adequately at the present time. Ignoring these two very large cases, the average differences from Schwartz's values in η, for both secant and cosecant normalizations, are 5.5% for S = 1 and 15.9% for S = 0.

Table I. List of present secant normalization values versus Schwartz's values for S = 1. The numbers in parentheses give the uncertainty in the last digit.

	Present		Schwartz	
k	$\tan(\eta)/k$	η(radians)	$\tan(\eta)/k$	η(radians)
0.1	-2.460(5)	-0.212(5)	-2.056(4)	-0.2028(4)
0.2	-2.555(5)	-0.472(1)	-2.260(3)	-0.4245(5)
0.3	-2.745(5)	-0.6880(9)	-2.492(4)	-0.6419(8)
0.4	-3.125(5)	-0.8960(8)	-2.833(2)	-0.84776(35)
0.5	-3.723(8)	-1.0778(9)	-3.384(3)	-1.0370(4)
0.6	-5.85(6)	-1.293(3)	-4.40(1)	-1.2087(7)
0.7	-8.35(2)	-1.4013(4)	-6.74(2)	-1.3619(6)
0.8	-28.75(5)	-1.52734(8)	-17.2(6)	-1.498(3)

Table II. List of present secant normalization values versus Schwartz's values for S = 0. The numbers in parentheses give the uncertainty in the last digit.

	Present		Schwartz	
k	$\tan(\eta)/k$	η(radians)	$\tan(\eta)/k$	η(radians)
0.1	-10.00(5)	-0.785(2)	-6.68(2)	-0.589(1)
0.2	-16.5(3)	-1.276(5)	-9.23(2)	-1.0743(9)
0.3	31.5(5)	1.465(2)	-26.4(1)	-1.4452(5)
0.4	8.15(5)	1.273(2)	15.87(4)	1.4145(4)
0.5	3.59(1)	1.062(1)	5.17(2)	1.2017(13)
0.6	2.135(1)	0.908(1)	2.845(8)	1.041(1)
0.7	1.455(1)	0.7946(3)	1.917(5)	0.9303(12)
0.8	1.10(2)	0.721(9)	1.530(5)	0.8857(16)

Table III. List of present cosecant normalization values versus Schwartz's values for S = 1. The numbers in parentheses give the uncertainty in the last digit.

	Present		Schwartz	
k	$-\mathrm{Cot}(\eta)/k$	η(radians)	$\mathrm{Tan}(\eta)/k$	η(radians)
0.1	41.920(5)	-0.23417(3)	-2.056(4)	-0.2028(4)
0.2	10.10(3)	-0.4597(12)	-2.260(3)	-0.4245(5)
0.3	4.1201(1)	-0.68023(1)	-2.492(4)	-0.6419(8)
0.4	2.0505(2)	-0.883859(5)	-2.833(2)	-0.84776(35)
0.5	1.09847(3)	-1.068541(11)	-3.384(3)	-1.0370(4)
0.6	0.572425(5)	-1.2399641(27)	-4.40(1)	-1.2087(7)
0.7	0.25708(6)	-1.39275(4)	-6.74(2)	-1.3619(6)
0.8	0.056993(7)	-1.525233(6)	-17.2(6)	-1.498(3)

Table IV. List of present cosecant normalization values versus Schwartz's values for S = 0. The numbers in parentheses give the uncertainty in the last digit.

	Present		Schwartz	
k	$-\mathrm{Cot}(\eta)/k$	η(radians)	$\mathrm{Tan}(\eta)/k$	η(radians)
0.1	11.245(3)	-0.72686(13)	-6.68(2)	-0.589(1)
0.2	1.6855(2)	-1.24566(4)	-9.23(2)	-1.0743(9)
0.3	-0.1188(1)	1.53517(3)	-26.4(1)	-1.4452(5)
0.4	-0.77845(2)	1.268932(7)	15.87(4)	1.4145(4)
0.5	-1.1076(2)	1.06504(7)	5.17(2)	1.2017(13)
0.6	-1.29527(3)	0.910137(11)	2.845(8)	1.041(1)
0.7	-1.39933(3)	0.79574(1)	1.917(5)	0.9303(12)
0.8	-1.409835(5)	0.725378(2)	1.530(5)	0.8857(16)

B. COMPARISON OF DIFFERENT NORMALIZATIONS

The average difference between the values of η calculated with secant and cosecant normalizations is 2%. One other observation is worthy of note, and that is that the values of $-\cot(\eta)/k$ found by the cosecant normalization have more apparent significant figures than the values of $\tan(\eta)/k$. This is due to the fact that the plots of $-\cot(\eta)/k$ versus k do not show fluctuations in $-\cot(\eta)/k$ anywhere as large as in $\tan(\eta)/k$. To see this compare Fig. 1 with Fig. 3. Since the normalization of the variational principle is arbitrary there should be no difference in accuracy from one to the other, and the comparison with Schwartz's results shows this to be true. Without Schwartz's results for comparison one would seem to have more confidence in the results of the cosecant normalization due to the larger number of apparent significant figures. However, without a standard of comparison, there is no reason why one normalization could not give more significant figures in a given case and still not give any better an answer for .

C. ACCURACY AND CONVERGENCE

The results examined above are for 40 terms in the sum and they show fairly good results for S = 1 and generally poorer results for S = 0. An examination of runs at $k = 0.4$ with 49, 56, and 72 terms shows the following. Beyond 40 convergence of the flat region toward Schwartz's values is very slow and not always guaranteed, since for the S = 0 secant normalization at 49 the value actually became worse. In addition, at 56 and 72 terms, significant errors in the matrix inversion were

noticed and the accuracy beyond about 50 terms became questionable. The limit imposed by computer accuracy was therefore between 50 and 60 terms, and within this limit continued convergence did not give appreciably better results.

D. RELATIVE ACCURACY OF S = 1 AND S = 0

The triplet (S = 1) calculation is better behaved than the singlet (S = 0) calculation, probably for the following reason: the anti-symmetric (triplet) Ψ is automatically 0 for $r_1 = r_2$ so that the electrons cannot coalesce. This effect is qualitatively the same as the effect of electrostatic repulsion, and thereby operates to remove some of the burden from the variational machinery. The singlet wave function contains no such built-in convenience. Thus for S = 1 the calculations have a greater absolute accuracy than for S = 0 and so should have a greater relative accuracy for S = 1 than for S = 0.

V. CONCLUSIONS

There are two differences between the trial functions used in this paper and those used by Schwartz. In the asymptotic part Schwartz used $\frac{\cos(kr_1)}{kr_1}\left(1-e^{-K/2r_1}\right)$ instead of $j_1(kr_1)$, and in the close-in terms Schwartz included an r_{12}^{ℓ} which was left out in the present calculations to make the integrals easier. From the comparison of the present results with Schwartz's results one concludes that in general the convergence of the curves for the present trial function is not as good in an equivalent number of terms. The idea that the effect on convergence of eliminating the r_{12}^{ℓ} factor could be offset by using more terms of a simpler form seems to be cut short by the inaccuracies in the matrix inversion and slower rates of convergence with larger numbers of terms. Therefore one concludes that a more complex trial function must be used to get good results, and that one can be misled by the apparently good accuracy (the small uncertainties in the tables) of the simpler trial functions without comparison. Finally one can conclude from the above comparison that the simpler form works reasonably well for $S = 1$ but not so well for $S = 0$, and that there is really no difference in accuracy between the two normalizations despite the larger number of apparent significant figures for the cosecant normalization.

APPENDIX A

THE VARIATIONAL PRINCIPLE

This appendix shows the steps in the derivation of the variational principle used, for the case of one radial coordinate r, and for the case of two radial coordinates r_1 and r_2.

1. One Radial Coordinate

Start with $I = \frac{2m}{\hbar^2}\int \Psi(E-\hat{H})\Psi \, d\tau$ where E is a constant energy term and $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(r)$

where U(r) is a central potential. Then write

$$\delta I = \frac{2m}{\hbar^2}\left[\int \delta\Psi(E-\hat{H})\Psi \, d\tau + \int \Psi(E-\hat{H})\delta\Psi \, d\tau\right]$$

Now using $$\Psi \nabla^2\delta\Psi \equiv \vec{\nabla}\cdot(\Psi\vec{\nabla}\delta\Psi) - \vec{\nabla}\cdot(\delta\Psi\nabla\Psi) + \delta\Psi\nabla^2\Psi$$

one gets $$\delta I = 2\frac{2m}{\hbar^2}\int \delta\Psi(E-\hat{H})\Psi \, d\tau + \int \vec{\nabla}\cdot(\Psi\vec{\nabla}\delta\Psi)\, d\tau - \int \vec{\nabla}\cdot(\delta\Psi\vec{\nabla}\Psi)\, d\tau .$$

Then $$\delta I = 2\frac{2m}{\hbar^2}\int \delta\Psi(E-\hat{H})\Psi \, d\tau + \int_S \Psi\vec{\nabla}\delta\Psi\cdot d\vec{S} - \int_S \delta\Psi\vec{\nabla}\Psi\cdot d\vec{S}$$

$$= 2\frac{2m}{\hbar^2}\int \delta\Psi(E-\hat{H})\Psi \, d\tau + \lim_{r\to\infty}\left[\int_S r^2\Psi\frac{d}{dr}\delta\Psi \, d\Omega - \int_S r^2\delta\Psi\frac{d}{dr}\Psi \, d\Omega\right]$$

since the integrals are over all space and $d\vec{S} = \hat{r}\, r^2 \, d\Omega$.

Finally $$\delta I = \lim_{r\to\infty}\int_S r^2\Psi\frac{d}{dr}\delta\Psi \, d\Omega - \lim_{r\to\infty}\int_S r^2\delta\Psi\frac{d}{dr}\Psi \, d\Omega$$

for Ψ exact. With Ψ properly normalized the integral over the angular part can be made unity. Then

$$\delta I = \lim_{r\to\infty}\left[R_\ell\, r^2\frac{d}{dr}\delta R_\ell - \delta R_\ell\, r^2\frac{d}{dr}R_\ell\right]$$

where R_ℓ is the radial portion of Ψ. Then inserting the condition

on R_ℓ at ∞

$$R_\ell \xrightarrow[r\to\infty]{} f(\eta_\ell)\ \frac{\sin(kr - \frac{\ell\pi}{2} + \eta_\ell)}{kr}$$

one finds, using $\delta R_\ell = \frac{\partial}{\partial \eta_\ell} R_\ell\ \delta\eta_\ell$

that $\delta I = -f^2(\eta_\ell)/k\ \delta\eta_\ell$ for exact. Note that in the case of one radial coordinate the correct normalization of Ψ for $\ell = 0$ is $\frac{1}{\sqrt{4\pi}}$.

2. Two Radial Coordinates

In this case $\hat{H} = \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + U(r_1, r_2, r_{12})$

Then as before

$$\delta I = \lim_{r_1\to\infty} \int_{\Omega_2}\int_{S_1} r_1^2 \Psi \frac{d}{dr_1}\delta\Psi\, d\Omega_1 d\tau_2 - \lim_{r_1\to\infty}\int_{\Omega_2}\int_{S_1} r_1^2 \delta\Psi \frac{d}{dr_1}\Psi\, d\Omega_1 d\tau_2$$
$$+ \lim_{r_2\to\infty}\int_{\Omega_1}\int_{S_2} r_2^2 \Psi \frac{d}{dr_2}\delta\Psi\, d\Omega_2 d\tau_1 - \lim_{r_2\to\infty}\int_{\Omega_1}\int_{S_2} r_2^2 \delta\Psi \frac{d}{dr_2}\Psi\, d\Omega_2 d\tau_1$$

for Ψ exact. Again with Ψ properly normalized the integrals over $d\Omega_1 d\Omega_2$ and $d\Omega_2 d\Omega_1$ can be made unity so

$$\delta I = \lim_{r_1\to\infty}\int_0^\infty \left[r_1^2 R_\ell \frac{d}{dr_1}\delta R_\ell - r_1^2 \delta R_\ell \frac{d}{dr} R_\ell\right] r_2^2 dr_2 + \lim_{r_2\to\infty}\int_0^\infty \left[r_2^2 R_\ell \frac{d}{dr_2}\delta R_\ell - r_2^2 \delta R_\ell \frac{d}{dr_2} R_\ell\right] r_1^2 dr_1$$

Then inserting the conditions

$$R_\ell \xrightarrow[r_1\to\infty]{} f(\eta_\ell)\ \frac{\sin(kr_1 - \frac{\ell\pi}{2} + \eta_\ell)}{kr_1}\ e^{-r_2}, \quad R_\ell \xrightarrow[r_2\to\infty]{} f(\eta_\ell)\ \frac{\sin(kr_2 - \frac{\ell\pi}{2} + \eta_\ell)}{kr_2}\ e^{-r_1}$$

one gets $\delta I = -\frac{2}{4} f^2(\eta_\ell)/k\ \delta\eta_\ell$ where the $\frac{2}{4}$ can be eliminated by putting an additional factor of $\frac{2}{\sqrt{2}}$ in the normalization of Ψ. So finally $\delta I = -f^2(\eta_\ell)/k\ \delta\eta_\ell$ as before. Note that the correct normalization of Ψ for $\ell = 0$ is now $\frac{2}{4\pi\sqrt{2}}$.

APPENDIX B

THE HAMILTONIAN

Write $\hat{H}\Psi = \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\Psi + e^2\left(\frac{-1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}\right)\Psi = E\Psi$

then $\left[\frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) + e^2\left(\frac{-1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}\right)\right]\Psi = \left(\frac{\hbar^2 k'^2}{2m} - \frac{me^4}{2\hbar^2}\right)\Psi$

where $\frac{-me^4}{2\hbar^2}$ is the ground state energy of hydrogen. Therefore

$$\frac{2m}{\hbar^2}[E-\hat{H}]\Psi = \left[k'^2 - \frac{m^2e^4}{\hbar^4} + \nabla_1^2 + \nabla_2^2 + \frac{2me^2}{\hbar^2}\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right)\right]\Psi = 0$$

Then let $\rho_1 = \alpha r_1$, $\rho_2 = \alpha r_2$ where $\alpha = \frac{me^2}{\hbar^2}$ so when $\rho_1 = \rho_2 = 1$ $r = \frac{\hbar^2}{me^2}$ or one Bohr Radius. So

$$\left[k'^2 - \frac{m^2e^4}{\hbar^4} + \nabla_{\rho_1}^2\alpha^2 + \nabla_{\rho_2}^2\alpha^2 + \frac{2me^2\alpha}{\hbar^2}\left(\frac{1}{\rho_1} + \frac{1}{\rho_2} - \frac{1}{\rho_{12}}\right)\right]\Psi = 0$$

and dividing through by α^2 and setting $k^2 = \frac{k'^2}{\alpha^2} = \frac{k'^2\hbar^4}{m^2e^4}$

$$\left[k^2 - 1 + \nabla_{\rho_1}^2 + \nabla_{\rho_2}^2 + \frac{2me^2}{\alpha\hbar^2}\left(\frac{1}{\rho_1} + \frac{1}{\rho_2} - \frac{1}{\rho_{12}}\right)\right]\Psi = 0$$

Now $E = \frac{\hbar^2 k'^2}{2m} = \frac{me^4 k^2}{2\hbar^2} = k^2 R_0$ where R_0 is the Rydberg energy so k^2 measures energy in Rydberg units. Finally

$$\frac{2m}{\hbar^2}[E-\hat{H}] = k^2 - 1 + \nabla_{\rho_1}^2 + \nabla_{\rho_2}^2 + \frac{2}{\rho_1} + \frac{2}{\rho_2} - \frac{2}{\rho_{12}}$$

and for excitation to the first excited state $E = \frac{3}{4}R_0$ is required which implies $k^2 < \frac{3}{4}$ and $k < \sqrt{\frac{3}{4}} = .866$.

```
      IMPLICIT REAL*8(A-H,O-Z)
      INTEGER S(100,2),T(100,2)
      REAL*8 K(10),KAPPA(25),MTX(100,100),MTXI(100,100),LAMB
     1DA(2)
      DIMENSION R1(100),R2(100),C1(100),C2(100),N(5),P(2),PH
     1ASE(2)
      NIT = 5
      NOT = 6
      READ(NIT,400) NSET
  400 FORMAT(I4)
      READ(NIT,399)(N(I),I=1,NSET)
  399 FORMAT(I4)
      READ(NIT,401) NP,NK,NKAPPA
  401 FORMAT(3I4)
      READ(NIT,402)(K(I),I=1,NK)
  402 FORMAT(F10.4)
      READ(NIT,402)(KAPPA(I),I=1,NKAPPA)
      READ(NIT,402)(P(I),I=1,NP)
      N1=N(NSET)
    2 READ(NIT,102)(S(I,1),T(I,1),S(I,2),T(I,2),I=1,N1)
  102 FORMAT(4I4)
      DO 40 L1=1,NP
      DO 40 L2=1,NK
C CALCULATION OF INTEGRALS
      CALL BI(K(L2),B1,P(L1))
      CALL BII(K(L2),B2,P(L1))
      CALL BIII(K(L2),B3,P(L1))
      DO 40 M=1,NSET
      N1=N(M)
      WRITE(NOT,300) N1,P(L1),K(L2)
  300 FORMAT('1','CALCULATIONS FOR',' N = ',I4,4X,'P = ',F6.
     12,4X,'K = ',F10.4/)
      WRITE(NOT,100)
  100 FORMAT(//T26,'I',6X,'S(I)',4X,'T(I)'/)
      WRITE(NOT,200)(I,S(I,L1),T(I,L1),I=1,N1)
  200 FORMAT(T25,I4,4X,I4,4X,I4)
      WRITE(NOT,103)
  103 FORMAT(//T24,'KAPPA',14X,'TAN/K',15X,'PHASE',14X,'-COT
     1/K',15X,'PHASE'/)
      DO 40 L3=1,NKAPPA
      DO 3 I=1,N1
    3 CALL BI(S(I,L1),T(I,L1),K(L2),KAPPA(L3),R1(I),R2(I),P(
     1L1))
      DO 6 I=1,N1
      DO 6 J=1,I
      CALL MIJ(S(I,L1),T(I,L1),S(J,L1),T(J,L1),K(L2),KAPPA(L
     13),MTX(I,J),P(L1))
      IF(J.EQ.I) GO TO 6
      MTX(J,I)=MTX(I,J)
    6 CONTINUE
C MATRIX INVERSION AND SOLUTION OF M*C = -R
      CALL GAUS31(N1,0.0,MTX,MTXI,KER,100)
      DO 13 I=1,N1
      SUM1=0.0
      SUM2=0.0
      DO 12 J=1,N1
      TERM1=MTXI(I,J)*R1(J)
      TERM2=MTXI(I,J)*R2(J)
      SUM1=SUM1+TERM1
   12 SUM2=SUM2+TERM2
      C1(I)=-1*SUM1
   13 C2(I)=-1*SUM2
C CALCULATION OF W'S
      SUM1=0.0
      DO 14 I=1,N1
      TERM=C1(I)*R1(I)
   14 SUM1=SUM1+TERM
      W1=SUM1
```

```
      SUM1=0.0
      DO 15 I=1,N1
      TERM=C2(I)*R1(I)
   15 SUM1=SUM1+TERM
      W2=2*SUM1
      SUM1=0.0
      DO 16 I=1,N1
      TERM=C2(I)*R2(I)
   16 SUM1=SUM1+TERM
      W3=SUM1
C SECANT NORMALIZATION
      LAMBDA(1)=W1+B1-(W2+B2+1/K(L2))**2/(4*(W3+B3))
      PHASE(1)=DATAN(K(L2)*LAMBDA(1))
C COSECANT NORMALIZATION
      LAMBDA(2)=W3+B3-(W2+B2-1/K(L2))**2/(4*(W1+B1))
      PHASE(2)=DATAN(-1/(K(L2)*LAMBDA(2)))
      WRITE(NOT,201) KAPPA(L3),(LAMBDA(I),PHASE(I),I=1,2)
  201 FORMAT(T20,F10.4,4(4X,D16.8))
   40 CONTINUE
      END


      FUNCTION FACTRL(M)
      IMPLICIT REAL*8(A-H,O-Z)
      IF(M.LE.1) GO TO 2
      N = M-1
      PROD = M
      DO 1 I=1,N
    1 PROD = PROD*(M-I)
      FACTRL = PROD
      RETURN
    2 FACTRL = 1.0
      RETURN
      END


      FUNCTION SIGF(N,A,J,K,B,C)
      IMPLICIT REAL*8(A-H,C-Z)
      PROD = J
      IF(J.EQ.(K+1)) GO TO 2
      I = 1
    1 PROD = PROD*(J-I)
      IF((J-I).EQ.(K+1)) GO TO 2
      I = I+1
      GO TO 1
    2 TERM = PROD*A
      SUM = 0.0
      DO 3 M=1,N
      TERM = TERM*(K-M+1)*C/((J-M+1)*B)
    3 SUM = SUM+TERM
      SIGF = SUM
      RETURN
      END


      FUNCTION F1(A,B,L,M)
      IMPLICIT REAL*8(A-H,O-Z)
      NOT=6
      C1=DGAMMA(0.5D 00)
      C6=DFLOAT(L+M+1)
      C2=DGAMMA(C6)
      C3=DGAMMA(L+1.5D 00)
      C4=2.0**(L+1)
      E=0.5*(L+M+1)
      C5=B**L/(A**2+B**2)**E
      F=0.5*(L+1-M)
      G=0.5*(2*L+3)
      Z=B**2/(A**2+B**2)
      SUM=1.0
      TERM=1.0
      DO 1 I=1,70
      TERM=TERM*(E+I-1)*(F+I-1)*Z/((G+I-1)*I)
```

```
      IF(DABS(TERM/SUM).LT.1.0D-09) GO TO 3
    1 SUM=SUM+TERM
    2 WRITE(NOT,102)
  102 FORMAT(T26,'70 TERMS')
    3 F1=C1*C2*C5/(C3*C4)*SUM
      RETURN
      END

      SUBROUTINE RI(J,M,K,KAPPA,RI1,RI2,P)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 K,KAPPA
      DIMENSION F2(25),F3(25)
      A1=FACTRL(J+2)
      A2=FACTRL(M+2)
      C1=KAPPA+1
      C2=2*KAPPA+1
      M1=M+3
      M2=M+2
      J1=J+3
      J2=J+2
      IF(J-M)11,11,9
    9 DO 10 N=1,J1
      F2(N)=F1(C2,K,0,J+M+4-N)
   10 F3(N)=F1(C2,K,1,J+M+4-N)
      GO TO 13
   11 DO 12 N=1,M1
      F2(N)=F1(C2,K,0,J+M+4-N)
   12 F3(N)=F1(C2,K,1,J+M+4-N)
   13 SUM=0.0
      TERM=1.0/M1
      DO 1 N=1,M1
      TERM=TERM*(M1-N+1)/C1
    1 SUM=SUM+TERM*F2(N)
      TERM=1.0/J1
      DO 2 N=1,J1
      TERM=TERM*(J1-N+1)/C1
    2 SUM=SUM+P*TERM*F2(N)
      TERM=1.0/M2
      DO 3 N=1,M2
      TERM=TERM*(M2-N+1)/C1
    3 SUM=SUM-TERM*F2(N)
      TERM=1.0/J2
      DO 4 N=1,J2
      TERM=TERM*(J2-N+1)/C1
    4 SUM=SUM-P*TERM*F2(N)
      RI1=8*SUM/(2.0/KAPPA)**(J+M)
      SUM=0.0
      TERM=1.0/M1
      DO 5 N=1,M1
      TERM=TERM*(M1-N+1)/C1
    5 SUM=SUM+TERM*F3(N)
      TERM=1.0/J1
      DO 6 N=1,J1
      TERM=TERM*(J1-N+1)/C1
    6 SUM=SUM+P*TERM*F3(N)
      TERM=1.0/M2
      DO 7 N=1,M2
      TERM=TERM*(M2-N+1)/C1
    7 SUM=SUM-TERM*F3(N)
      TERM=1.0/J2
      DO 8 N=1,J2
      TERM=TERM*(J2-N+1)/C1
    8 SUM=SUM-P*TERM*F3(N)
      RI2=-8*(SUM+A2*F1(KAPPA,K,1,J)/C1**M1+P*A1*F1(KAPPA,K,
     11,M)/C1**J1)/(2.0/KAPPA)**(J+M)
      RETURN
      END

      SUBROUTINE MIJ(J,M,P,C,K,KAPPA,MTXIJ,S)
      IMPLICIT REAL*8(A-H,O-Z)
```

```
      INTEGER P,Q
      REAL*8 K,KAPPA,MTXIJ
      A1=FACTRL(J+P+2)
      A2=FACTRL(M+Q+2)
      A3=FACTRL(J+Q+2)
      A4=FACTRL(M+P+2)
      C1= 2*KAPPA
      C2= 4*KAPPA
      N1= M+Q+J+P+5
      N2= M+Q+J+P+4
      N3= M+Q+J+P+6
      F1= C1**N1
      F2= C2**N1
      F3= C1**N2
      F4= C1**N3
      S1= SIGF(M+Q+3,A2,N2,M+Q+3,C1,C2)/F2
      S2= SIGF(J+P+3,A1,N2,J+P+3,C1,C2)/F2
      S3= SIGF(M+P+3,A4,N2,M+P+3,C1,C2)/F2
      S4= SIGF(J+Q+3,A3,N2,J+Q+3,C1,C2)/F2
      T1= (2*(K**2-1)+4*KAPPA**2)*(A1*A2+S*A3*A4)/F4
      T2=(-4*KAPPA*(P+1))*(A1*A2/(J+P+2)+S*A3*A4/(M+P+2))/F1
      T3=(-4*KAPPA*(Q+1))*(A1*A2/(M+Q+2)+S*A3*A4/(J+Q+2))/F1
      T4= 2*P*(P+1)*(A1*A2/((J+P+2)*(J+P+1))+S*A3*A4/((M+P+2
     1)*(M+P+1)))/F3
      T5= 2*Q*(Q+1)*(A1*A2/((M+Q+2)*(M+Q+1))+S*A3*A4/((J+Q+2
     1)*(J+Q+1)))/F3
      MTXIJ=2*(T1+T2+T3+T4+T5+4*S1+4*S2+4*S*S3+4*S*S4)/(2.0/
     1KAPPA)**(J+M+P+Q)
      RETURN
      END


      SUBROUTINE BI(K,B1,P)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 K
      NOT=6
      A1=K**2
      A2=1+A1
      A3=1-A1
      A4=A2**2
      A5=A2**3
      T1=4/A5
      T2=4*A3/(A1*A4)
      T3=6*A3/(A1*A5)
      T4=2/(A1*A2)
      TERM=1.0
      SUM=TERM
      DO 1 N=2,70
      F1=(N**2-1.0)/N**2
      TERM=-1*TERM*F1*A1
      IF(DABS(TERM/SUM).LT.1.0D-09) GO TO 3
    1 SUM=SUM+TERM
    2 WRITE(NOT,102)
    3 B1=SUM-P*T1+P*T2-P*T3+P*T4
  102 FORMAT(T26,'B1 DOES NOT CONVERGE IN 70 TERMS')
      RETURN
      END


      SUBROUTINE BII(K,B2,P)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 K
      NOT=6
      A1=K**2
      A2=1+A1
      A3=1-A1
      A4=1+3*A1
      A5=K**3
      A6=A2**2
      A7=A2**3
      T1=1/K
      T2=8*A3/(K*A7)
```

```
      T3=8*K/A7
      T4=12*A1/(A5*A6)
      T5=4*A4/(A5*A7)
      T6=4/(A5*A2)
      T7=4/(K*A6)
      TERM1=5*K/6
      TERM2=4*A3/(K*A6)
      TERM3=16*K/(3*A6)
      SUM1=TERM1
      DO 1 N=3,70
      F2=(N-1.0)**2*(2.0*N+1.0)*(2.0*N-3.0)/((2.0*N-1.0)**2*
     1(N-2.0)*N)
      TERM1=-1*TERM1*F2*A1
      IF(DABS(TERM1/SUM1).LT.1.0D-09)GO TO 3
    1 SUM1=SUM1+TERM1
    2 WRITE(NOT,102)
    3 SUM=TERM2+TERM3
      DO 4 N=2,70
      F3=(N-1.0)/N
      F4=(2.0*N-1.0)/(2.0*N+1.0)
      TERM2=-1*TERM2*F3*A1
      TERM3=-1*TERM3*F4*A1
      TERM=TERM2+TERM3
      IF(DABS(TERM/SUM).LT.1.0D-09) GO TO 6
    4 SUM=SUM+TERM
    5 WRITE(NOT,102)
    6 B2=-1*(SUM1+P*SUM+T1-P*T2-P*T3+P*T4-P*T5+P*T6-P*T7)
  102 FORMAT(T26,'B2 DOES NOT CONVERGE IN 70 TERMS')
      RETURN
      END

      SUBROUTINE BIII(K,B3,P)
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 K
      NOT=6
      A1=K**2
      A2=1+A1
      A3=1+3*A1
      A4=2*A1
      A5=2+14*A1
      A6=A2**2
      A7=A2**3
      T1=3.141593/(3*K)
      T2=4/A7
      T3=6/(A1*A2)
      T4=A5/(A1*A7)
      T5=8/(A1*A6)
      T6=8/A6
      TERM1=A1/4
      SUM1=TERM1
      DO 1 N=3,70
      F5=(N-1.0)**2/((N-2.0)*N)
      TERM1=-1*TERM1*F5*A1
      IF(DABS(TERM1/SUM1).LT.1.0D-09) GO TO 3
    1 SUM1=SUM1+TERM1
    2 WRITE(NOT,102)
    3 TERM3=4*A3/(A1*A6)
      TERM4=8*A4/(3*A6)
      SUM=TERM3+TERM4
      DO 7 N=2,70
      F3=(N-1.0)/N
      F4=(2.0*N-1.0)/(2.0*N+1.0)
      TERM3=-1*TERM3*F3*A1
      TERM4=-1*TERM4*F4*A1
      TERM=TERM3+TERM4
      IF(DABS(TERM/SUM).LT.1.0D-09)GO TO 9
    7 SUM=SUM+TERM
    8 WRITE(NOT,102)
    9 B3=SUM1+P*SUM+T1+P*T2+P*T3-P*T4-P*T5-P*T6
  102 FORMAT(T26,'B3 DOES NOT CONVERGE IN 70 TERMS')
      RETURN
```

```
      END

      SUBROUTINE GAUS31(N,EPS,A,X,KER,K)
      REAL*8 A,X,Y,D
      DIMENSION A(1),X(1),L(100),M(100),Y(100,100)
      DO 1 I=1,N
      DO 1 J=1,N
      IND=(I-1)*K+J
    1 Y(I,J)=A(IND)
      KER=1
      N2=2*N
      CALL ARRAY1(2,N,N,100,100,Y,Y)
      CALL MINV1(Y,N,D,L,M)
      CALL ARRAY1(1,N,N,100,100,Y,Y)
      IF(D.EQ.0.) KER=2
      DO 2 I=1,N
      DO 2 J=1,N
      IND=(I-1)*K+J
    2 X(IND)=Y(I,J)
      RETURN
      END

      SUBROUTINE ARRAY1(MODE,I,J,N,M,S,D)
      DIMENSION S(1),D(1)
      REAL*8 S,D
      NI=N-I
      IF(MODE-1) 100,100,120
  100 IJ=I*J+1
      NM=N*J+1
      DO 110 K=1,J
      NM=NM-NI
      DO 110 L=1,I
      IJ=IJ-1
      NM=NM-1
  110 D(NM)=S(IJ)
      GO TO 140
  120 IJ=0
      NM=0
      DO 130 K=1,J
      DO 125 L=1,I
      IJ=IJ+1
      NM=NM+1
  125 S(IJ)=D(NM)
  130 NM=NM+NI
  140 RETURN
      END

      SUBROUTINE MINV1(A,N,D,L,M)
      DIMENSION A(1),L(1),M(1)
      DOUBLE PRECISION A,D,BIGA,HOLD
      D=1.0
      NK=-N
      DO 80 K=1,N
      NK=NK+N
      L(K)=K
      M(K)=K
      KK=NK+K
      BIGA=A(KK)
      DO 20 J=K,N
      IZ=N*(J-1)
      DO 20 I=K,N
      IJ=IZ+I
   10 IF(DABS(BIGA)-DABS(A(IJ))) 15,20,20
   15 BIGA=A(IJ)
      L(K)=I
      M(K)=J
   20 CONTINUE
      J=L(K)
      IF(J-K) 35,35,25
```

```
 25 KI=K-N
    DO 30 I=1,N
    KI=KI+N
    HOLD=-A(KI)
    JI=KI-K+J
    A(KI)=A(JI)
 30 A(JI)=HOLD
 35 I=M(K)
    IF(I-K) 45,45,38
 38 JP=N*(I-1)
    DO 40 J=1,N
    JK=NK+J
    JI=JP+J
    HOLD=-A(JK)
    A(JK)=A(JI)
 40 A(JI)=HOLD
 45 IF(BIGA) 48,46,48
 46 D=0.0
    RETURN
 48 DO 55 I=1,N
    IF(I-K) 50,55,50
 50 IK=NK+I
    A(IK)=A(IK)/(-BIGA)
 55 CONTINUE
    DO 65 I=1,N
    IK=NK+I
    IJ=I-N
    DO 65 J=1,N
    IJ=IJ+N
    IF(I-K) 60,65,60
 60 IF(J-K) 62,65,62
 62 KJ=IJ-I+K
    A(IJ)=A(IK)*A(KJ)+A(IJ)
 65 CONTINUE
    KJ=K-N
    DO 75 J=1,N
    KJ=KJ+N
    IF(J-K) 70,75,70
 70 A(KJ)=A(KJ)/BIGA
 75 CONTINUE
    A(KK)=1.0/BIGA
 80 CONTINUE
    K=N
100 K=K-1
    IF(K) 150,150,105
105 I=L(K)
    IF(I-K) 120,120,108
108 JQ=N*(K-1)
    JR=N*(I-1)
    DO 110 J=1,N
    JK=JQ+J
    HOLD=A(JK)
    JI=JR+J
    A(JK)=-A(JI)
110 A(JI)=HOLD
120 J=M(K)
    IF(J-K) 100,100,125
125 KI=K-N
    DO 130 I=1,N
    KI=KI+N
    HOLD=A(KI)
    JI=KI-K+J
    A(KI)=-A(JI)
130 A(JI)=HOLD
    GO TO 100
150 RETURN
    END
```

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13. ABSTRACT

The Kohn variational method of calculating scattering phase shifts has been examined previously, and calculations of the phase shifts of S-wave electrons on atomic hydrogen done, by Schwartz. This paper presents the results of using a trial function somewhat simpler than Schwartz's and compares the two sets of results. In addition this paper presents and compares the results of two different normalizations of the variational principle and gives a somewhat more detailed development of the variational principle used than in most previous papers.

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